Chloranil

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 7.44

Global applicability domain: Inside

Local applicability domain index: 9.68e-01

Confidence level: 8.59e-01

Nearest Neighbors from the Training Set

Image not found
Benzene, bromophenoxy-
Measured: 7.24
Predicted: 7.44

Image not found
1,2,3-Trichloronaphthalene
Measured: 7.66
Predicted: 7.45